Disposal System Material Properties

Fuel Cycle Research & Development

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Appendix E
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CONTENTS

TABLES

ACRONYMS

THMC	thermal-hydraulic-mechanical-chemical
DRZ	disturbed rock zone
CEC	cation exchange capacity

1. Introduction

Modeling of thermal-hydrological-mechanical-chemical (THMC) processes requires extensive parameter inputs to support process relationships for thermal, hydrological, mechanical, and chemical processes, as well as some additional parameters to support coupling of these processes. The parameters needed depend in part on the process models to be used. Therefore, a discussion of the models that are expected to be used is in order.

Data are provided for two argillaceous formations that have been intensively investigated for nuclear waste disposal: the Opalinus Clay at Mont Terri, Switzerland and the Boom Clay at Mol, Belgium. The Opalinus Clay is an indurated, stiff clay whereas the Boom Clay is a soft, plastic clay formation. Note that a range of values is presented where available but for some parameters only a best estimate or average value is available. Many of the parameters are also functions of thermodynamic conditions (e.g., temperature, pressures, composition) however these functional dependencies are not quantified in this report. Instead, the parameters are mainly reported at ambient conditions for the underground laboratories, or in some cases at generic standard conditions. In addition, rock and fluid parameters will generally be spatially variable, which is not addressed in this report. Spatial variability may require representing these parameters as a function of position.

2. Hydrologic Model

Hydrologic parameters for the Opalinus Clay and Boom Clay are given in Tables 1 through 3. The near-field, where THMC processes are most critical, also must consider the fact that an argillaceous host rock may have a fracture network within the disturbed rock zone (DRZ). Whether a dual-continuum approach or a discrete fracture network approach is used, hydrological properties are needed for the fractures and for the rock (matrix). The near-field rock will also likely be unsaturated for some time period following repository closure. Therefore, unsaturated flow parameters are also needed. The parameters in Table 2 are specifically for a dual-continuum approach. This is used now because specific parameters for a discrete fracture approach are still in development. The choice mainly impacts fracture geometry parameterization, which for a discrete fracture model would have additional parameters. Fracture geometry in the continuum model is defined by the fracture porosity and interface area per unit volume. A non-Newtonian flow parameter, as described in Liu et al. (2011), is also included in Table 1 however this parameter has not been evaluated for flow data from the Opalinus Clay or Boom Clay. Because hydrologic parameters can be, and generally are, spatially variable, the database needs to be able to accommodate spatial dependence of the parameters. For the Opalinus clay, bedding planes result in anisotropic behavior represented by parameterization parallel and perpendicular to bedding, such as hydraulic conductivity in Table1. This anisotropy is less pronounced for the Boom Clay (Bertrand, et al., 2009, Section 4.3.1).

Note that only limited fracture data is currently available for the Opalinus Clay and the Boom Clay and these data pertain to the DRZ around repository excavations. There are indications from the geologic record that natural fractures and flow processes through natural fracture pathways in argillaceous rock is possible (Cosgrove 2001; Arnould 2006). However, this information also indicates that fractures and associated flow processes are transient and that any record of fractures or flow through fractures can be difficult to identify. Hydrological parameters for two-phase flow in fractures are not available for the Opalinus Clay and Boom Clay. These parameters include the same parameter types as given in Table 2 for rock plus the active fracture parameter that quantifies preferential flow effects in fracture networks (Liu et al., 1998).

Table 1. Hydrologic: Single-phase properties for rock matrix

Property	Opalinus Clay	Boom Clay
Total porosity (HTO) (-)	0.14 – 0.247[1]	0.30 – 0.40[2]
Geochemical porosity (Cl^-, I^-) (-)	0.08 – 0.10[1]	0.12 – 0.25[3]
Grain density ($kg\text{-}m^{-3}$)	2700 – 2770[1]	2600 – 2670[4]
Hydraulic conductivity parallel to bedding ($m\text{-}s^{-1}$)	2e – 13[1]	2e-12 – 5e-12[2]
Hydraulic conductivity perpendicular to bedding ($m\text{-}s^{-1}$)	4e – 14[1]	
Specific Storativity (m^{-1})	1e-7 – 1e-4[1]	7e-5 – 2e-4[8]
Non-Newtonian (non-Darcy) flow parameter[5]	NA	NA
Dispersivity (m)	0.12 – 0.2[6]	0.004[7]

1. Bossart (2012, Pages 4-17 and 4-19); 2. Shaw (2010, Table 1) 3. ONDRAF/NIRAS (2001, Section 11.3.8.2.3) and Aertsens et al. (2003, p. 433); 4. Shaw (2010, Table 1) and Aertsens et al. (2003, p. 432); 5. Liu et al. (2011, Section 2.2); 6. Zheng et al. (2007, p. 369) and De Windt et al. (2004, Table 1); 7. Martens et al. (2008, Table 4); 8. Based on Bernier and Neerdael (1996) value of 0.95 m^2/yr hydraulic diffusivity, with specific storativity computed from hydraulic conductivity divided by hydraulic diffusivity.
NA = not available

Table 2. Hydrologic: Two-phase properties for rock matrix

Property	Opalinus Clay	Boom Clay
rock van Genuchten pore size distribution index, m (-)	0.33 – 0.5[2]	0.3[1]
rock van Genuchten capillary strength α (Pa^{-1})	4.8e-8 – 2.0e-7[2]	2.9e-7[1]
rock residual aqueous saturation (-)	0 – 50%[2]	20%[3]
rock residual gas saturation (-)	0 – 5%[2]	17.4%[3]
aqueous-gas interfacial tension (Pa-m) (at natural temperature – see Table 4)	0.074[4]	0.073[4]
aqueous-gas-mineral contact angle (°)	NA	NA

1. Shaw et al. (2010); 2. Johnson (2004, p. 44); 3. Dymitrowska et al. (2009, p. 20, Table 3); 4. Batchelor (1967, Appendix1)
NA = not available

Table 3. Hydrologic: Single-phase properties for fractures

Property	Opalinus Clay	Boom Clay
DRZ fracture porosity (porosity of fracture domain) (-)	NA	NA
DRZ fracture grain density ($kg\text{-}m^{-3}$)	NA	NA
DRZ fracture conductivity maximum ($m\text{-}s^{-1}$)	2e-8 – 2e-5[1]	2e-11 – 5e-11[2]
DRZ fracture interface area per unit volume (m^{-1})	NA	NA
Dispersivity (m)	NA	NA

1. Bossart (2004, p. 437); 2. Yu et al. (2011, p. 31 – indicates one order of magnitude damage, which has been applied to matrix conductivity values from Table 1)
NA = not available

Tables 4 and 5 provide physical fluid property parameters relevant to natural conditions for the Opalinus Clay and Boom Clay. The database needs to be able to accommodate temperature and, in some cases, pressure and compositional dependence of these parameters.

Table 4. Aqueous Phase: Physical Properties and Conditions

Property	Opalinus Clay	Boom Clay
natural temperature (°C)	13 – 15[1]	16[2]
viscosity (Pa-s) (at natural temperature)	1.14e-3 – 1.20e-3[3]	1.11e-3[3]
density (kg-m^{-3}) (at natural temperature and TDS level – see Table 10)	1013[4]	1000[4]
dielectric constant (relative permittivity) (-)(at natural temperature)	78[5]	82[5]

1. Degueldre et al. (2003, Table 4); 2. DeCraen et al. (2004, Table 1-1); 3. Batchelor (1967, Appendix1) ; 4.Fischer et al. (1979, Appendix 1) ; 5. Klein and Swift (1977, Figure 3)

Table 5. Gas phase – Moist Air (100% relative humidity): Physical Properties

Property	Opalinus Clay	Boom Clay
viscosity (Pa-s) (at natural temperature – see Table 4 – and atmospheric pressure)	1.8e-5[1]	1.8e-5[1]
density (kg-m^{-3}) (at natural temperature – see Table 4 – and atmospheric pressure)	1.2[1]	1.2[1]

1. Tsilingiris (2008, Figures 1 and 2)

3. Mechanical Model

Mechanical models for THMC processes in clay host rock are currently based on elasticity theory for rock, supplemented with coupling terms to account for water saturation and aqueous compositional effects on swelling clays. Parameter values for the Opalinus Clay and the Boom Clay are provided in Tables 6 through 9. The elasticity theory has also been expanded upon for a dual-domain situation, as described in Liu et al., (2010; 2011), in which there is a “hard part” that only experiences small deformations and a “soft part” that can experience large deformations. Conceptually, the “hard part” and “soft part” roughly correspond to the rock matrix and fractures, respectively. The parameters for the mechanical model and for coupling with hydrological conditions are given in Table 8. Because rock mechanical parameters can be, and generally are, spatially variable, the database needs to be able to accommodate spatial dependence of the parameters. For the Opalinus clay, bedding planes result in anisotropic mechanical properties represented by parameterization parallel and perpendicular to bedding. This anisotropy is not as pronounced for the Boom Clay.

Table 6. Mechanical: Elastic properties

Property	Opalinus Clay	Boom Clay
Young's modulus – perpendicular to bedding (MPa)	2100 – 3500[1]	300 – 400[2]
Young's modulus – parallel to bedding (MPa)	6300 – 8100[1]	
Poisson's ratio – perpendicular to bedding	0.28 – 0.38[1]	0.125 – 0.45[2]
Poisson's ratio – parallel to bedding	0.16 – 0.32[1]	
Shear Modulus (MPa)	800 – 1600[1]	40[3]
Uniaxial tensile strength perpendicular to bedding (MPa)	1[1]	0.1[3**]
Uniaxial tensile strength parallel to bedding (MPa)	2[1]	
Uniaxial compressive strength perpendicular to bedding (MPa)	23.1 – 28.1[1]	2.2[3**]
Uniaxial compressive strength parallel to bedding (MPa)	4.0 – 17.0[1]	
Young’s modulus soft part (MPa)	0.6 – 3.6[4]	NA
Young’s modulus hard part (MPa)	2080 – 3345[4]	NA
Volume fraction soft part (-)*	0.00036 – 0.0048[4]	NA
Volume fraction hard part (-)*	0.9952 – 0.99964[4]	NA

1. Bossart (2012, p. 4-4); 2. Shaw (2010, Table 1); 3. Dehandshutter et al. (2005, Table 1); 4. Liu et al. (2011, Table 2-1);
NA = not available

*Note: volume fractions of hard and soft parts add to 1.

** Marked as questionable by Dehandshutter et al. (2005, Table 1).

Table 7. Mechanical: Plasticity

Property	Opalinus Clay	Boom Clay
Plastic limit (%)	21 – 25[1]	22 – 28[2]
Liquid limit (%)	33 – 43[1]	59 – 83[2]

1. Martin and Lanyon (2003, Table 1); 2. Shaw (2010, Table 1)

Table 8. Mechanical: Mohr-Coulomb-Griffith Failure and Moisture Coupling Properties

Property	Opalinus Clay	Boom Clay
Cohesive strength (MPa)	2.2 – 5.5[1]	0.175 – 0.300[2]
Friction angle (°)	24 – 26[1]	18[2]
Yield stress (MPa)	20 – 22[5]	NA
Swelling pressure (MPa)*	5.5[4]	0.6[3]
Swelling strain (axial, %)*	7.5[4]	5 – 10[3]
Swelling strain (radial, %)*	2[4]	NA
Swelling strain (volumetric, %)*	11.5[4]	NA
Swelling pressure perpendicular to bedding (MPa)**	1.2[1]	NA
Swelling pressure parallel to bedding (MPa)**	0.5[1]	NA
Swelling strain perpendicular to bedding (%)**	5 – 9[1]	NA
Swelling strain parallel to bedding (%)**	0.5 – 2.0[1]	NA

1. Bossart (2012, p. 4-21 to 4-23); 2. Dehandshutter et al. (2005, Table 1); 3. Bernier et al. (1997, Figures 14 and 15). 4. Zhang et al. (2010, p. 48-49); 5. Horseman et al. (2005, Figure 20)
NA = not available

*Note that the swelling tests reported by Bernier et al. (1997) for the Boom Clay were conducted by controlling relative humidity, which ranged over a complete wetting-drying cycle. Since water was introduced as a vapor, it would also be free of dissolved constituents. Therefore, the swelling data for the Boom Clay represent swelling caused by altering water composition and water content. The swelling data reported by Zhang et al. (2010) for the Opalinus Clay also were measured through controlling capillary pressure through relative humidity and are comparable with those reported by Bernier et al. (1997) for the Boom Clay.

** Note that the swelling tests for the Opalinus Clay reported by Bossart (2012, page 4-23) are conducted using IRSM standard methods. Undisturbed samples that have their native water content are used for the test (Madsen, 1999, page 294). These samples are immersed in distilled water to determine the swelling pressure for confined conditions or swelling strain if unconfined. Because undisturbed samples should be saturated, this test provides information on the effects of changing aqueous composition on swelling stress and strain. It is not clear from the presentation, however, whether swelling strain represents volumetric, axial, or radial strain.

Table 9. Mechanical: In-Situ Conditions

Property	Opalinus Clay	Boom Clay
Maximum stress (MPa)	6 – 7[1]	4.5[2]
Maximum stress direction (trend, plunge)(°)	210, 70[1]	vertical
Intermediate stress (MPa)	4 – 5[1]	1.4 – 4.1[2]
Intermediate stress direction (trend, plunge)(°)	320, 10[1]	horizontal
Minimum stress (MPa)	0.6 – 2[1]	1.4 – 4.1[2]
Minimum stress direction (trend, plunge)(°)	50, 15[1]	horizontal
Pore pressure (MPa)	1 – 2[1]	2.2[2]
Overconsolidation ratio (OCR) (-)	2.5 – 4.8[5,6]	1 – 2.4[3,4]

1. Martin and Lanyon (2003, p. 1085 and 1087); 2. Bernier et al. (2007, p. 230); 3. Mertens et al. (2003, p. 310) - The minimum OCR for the Boom Clay is an apparent OCR based on the current overburden being the same as the maximum; 4. Shaw (2010, Table 3). 5. Lemy et al. (2006, p. 3) 6. The maximum OCR for the Opalinus Clay is an apparent OCR based on a current overburden of 280 m and a maximum overburden of 1350 m (Bossart, 2012, p. 4-11).

4. Chemical Model

The current chemical model involves aqueous complexation, cation exchange, and mineral precipitation/dissolution. Other site-specific information includes aqueous chemical composition, specific surface areas, and diffusion and sorption parameters. The parameters for chemical processes are given in Tables 10 through 17.

Table 10. Aqueous: Chemical Composition

Property	Opalinus Clay	Boom Clay
pH (–log[H$^+$])	7.3 – 7.96[1]	8.5[2]
Eh (mV)	-227[1]	-274[2]
Ionic strength (mol-L^{-1})	0.350[1]	0.016[2]
Mineralization TDS (total dissolved solids) (mg-L^{-1})	18,296[1]	935[3]
Alkalinity (mEq-L^{-1})	0.749 –2.5[1]	15.12[2]
Total organic carbon (TOC) (mg-L^{-1} as carbon)	14[1]	150[4]
Total inorganic carbon (TIC) (mg-L^{-1} as carbon)	8.5[1]	181.3[2]
pCO$_2$ (log bars)	-3.58 to -2.69[1]	-2.62[2]
Ca (mg-L^{-1})	609.0[1]	2.0[2]
Li (mg-L^{-1})	0.4[1]	NA
Na (mg-L^{-1})	5640[1]	359[2]
Mg (mg-L^{-1})	415.0[1]	1.6[2]
K (mg-L^{-1})	43.4[1]	7.2[2]
Fe (mg-L^{-1})	0.14[1]	0.2[2]
Al (mg-L^{-1})	0.013[1]	0.6e-3[2]
Si (mg-L^{-1})	1.61[1]	3.4[2]
NH$_4$ (mg-L^{-1})	10.2[1]	NA
Ba (mg-L^{-1})	0.019[1]	NA
B (mg-L^{-1})	1.61[1]	NA
Mn (mg-L^{-1})	0.346[1]	NA
Sr (mg-L^{-1})	35.00[1]	NA
Cl (mg-L^{-1})	10,170[1]	26[2]
SO$_4$ (mg-L^{-1})	1,320[1]	2.2[2]
Br (mg-L^{-1})	35.0[1]	0.6[4]
HCO$_3$ (mg-L^{-1})	NA	878.9[2]
I (mg-L^{-1})	2.2[1]	NA
NO$_3$ (mg-L^{-1})	10.0[1]	NA
NO$_2$ (mg-L^{-1})	2.0[1]	NA
F (mg-L^{-1})	0.75[1]	3[4]

1. Bossart (2012, p. 4-14 to 4-16); 2. Li et al. (2007, Table 4.2); 3. DeCraen (2006, p. 7); 4. DeCraen et al. (2006, Table 3)
NA = not available

A database of thermodynamic parameters that include equilibrium constants, molecular weights of aqueous species and minerals, parameters for calculating activity coefficients, molar volumes of minerals is required. A standard database for chemical equilibria is the EQ3/6V7.2b database. This information is too voluminous to present here, so the general citation to Wolery (1992) is used. This information is site-specific to the extent that the speciation, compositions, and thermodynamic conditions that are applicable to the Opalinus Clay and Boom Clay are adequately represented.

Table 11. Chemical Reaction: Chemical Equilibrium Parameters

Property	Opalinus Clay	Boom Clay
Equilibrium constants (dimensions are reaction dependent)	Wolery (1992)	Wolery (1992)

Chemical kinetic parameters for a model of the Opalinus Clay are given in Liu et al. (2011, Table 4-7) and is reproduced here in Table 12. Similar parameters should also apply to the Boom Clay, but specific information for this formation is not available.

Table 12. Chemical Reaction: Chemical Kinetic Parameters for Opalinus Clay, (Liu et al., 2011, Table 4-7)

Mineral	A (cm^2-g^{-1})	**Parameters for Kinetic Rate Law**							
		Neutral Mechanism		**Acid Mechanism**			**Base Mechanism**		
		k_{25} (mol-$m^{-2}s^{-1}$)	**E_a (KJ-mol^{-1})**	**k_{25} (mol-$m^{-2}s^{-1}$)**	**E_a (KJ-mol^{-1})**	**$n(H^+)$**	**k_{25} (mol-$m^{-2}s^{-1}$)**	**E_a (KJ-mol^{-1})**	**$n(H^+)$**
***Primary*:**									
Calcite	Assumed at equilibrium								
Quartz	9.8	1.023×10^{-14}	87.7						
K-feldspar	9.8	3.89×10^{-13}	38	8.71×10^{-11}	51.7	0.5	6.31×10^{-12}	94.1	-0.823
Kaolinite	1.95×10^{5}	6.91×10^{-14}	22.2	4.89×10^{-12}	65.9	0.777	8.91×10^{-18}	17.9	-0.472
Illite	6.68×10^{5}	1.66×10^{-13}	35	1.05×10^{-11}	23.6	0.34	3.02×10^{-17}	58.9	-0.4
Chlorite	9.8	3.02×10^{-13}	88	7.76×10^{-12}	88	0.5			
Dolomite	12.9	2.52×10^{-12}	62.76	2.34×10^{-7}	43.54	1			
Ankerite	9.8	1.26×10^{-9}	62.76	6.46×10^{-4}	36.1	0.5			
Smectite-Na	5.64×10^{5}	1.66×10^{-13}	35	1.05×10^{-11}	23.6	0.34	3.02×10^{-17}	58.9	-0.4
Na-montmorillonite	5.64×10^{5}	1.66×10^{-13}	35	1.05×10^{-11}	23.6	0.34	3.02×10^{-17}	58.9	-0.4

Note: k_{25} = kinetic rate parameter at 25° C, E_a = activation energy, $n(H^+)$ = power term (Xu et al., 2006, Table 8)

Additional parameters are needed if transport processes involving dissolved species are to be included in the model. These parameters relate to diffusion and dispersion phenomena and to sorption interactions between aqueous species and mineral surfaces. The database needs to be able to accommodate spatial dependence of these parameters.

Table 13. Aqueous: Diffusion Coefficient

Property	Opalinus Clay	Boom Clay
H(HTO) (m^2-s^{-1}) parallel to bedding	4e-11 – 1e-10[1]	1.1e-10 – 5.5e-10[2]
H(HTO) (m^2-s^{-1}) perpendicular to bedding	1e-11 – 2e-11[1]	
H(HTO) accessible porosity (%)	15 – 17[1]	34 – 40[2]
I^- (m^2-s^{-1}) parallel to bedding	8.0e-12 – 3.0e-11[1]	9.1e-11 – 5.2e-10[2]
I^- (m^2-s^{-1}) perpendicular to bedding	2.4e-12 – 4.2e-12 [1]	
I^- accessible porosity (%)	5 – 15[1]	14 – 18[2]
Cl^- (m^2-s^{-1}) parallel to bedding	1.8e-11 – 6.8e-11[1]	NA
Cl^- (m^2-s^{-1}) perpendicular to bedding	4.8e-12[1]	NA
Cl^- accessible porosity (%)	6 – 12[1]	NA
Br^- (m^2-s^{-1}) parallel to bedding	1.7e-11 – 4.5e-11[1]	NA
Br^- accessible porosity (%)	10 – 15[1]	NA
Cs^+ (m^2-s^{-1}) parallel to bedding	2.6e-10 – 2.7e-10[1]	NA
Cs^+ accessible porosity (%)	17 – 18[1]	NA
$^{22}Na^+$ (m^2-s^{-1}) parallel to bedding	7.2e-11[1]	NA
$^{22}Na^+$ accessible porosity (%)	17 – 18[1]	NA
$^{85}Sr^{2+}$(m^2-s^{-1}) parallel to bedding	6.5e-11 – 7.0e-11[1]	NA
$^{85}Sr^{2+}$ accessible porosity (%)	15 – 17[1]	NA
$^{60}Co^{2+}$ (m^2-s^{-1}) parallel to bedding	6.0e-11[1]	NA
$^{60}Co^{2+}$ accessible porosity (%)	15[1]	NA
$^{6}Li^+$ (m^2-s^{-1}) parallel to bedding	7.0e-11[1]	NA
$^{6}Li^+$ accessible porosity (%)	16[1]	NA
SeO_4^{2-} (m^2-s^{-1})	NA	1.5e-11 – 7.3e-11[3]
SeO_4^{2-} accessible porosity (%)	NA	5 – 18[3]
HSe^- (m^2-s^{-1})	NA	8e-11 – 1.7e-10[3]
HSe^- accessible porosity (%)	NA	12 – 18[3]

1. Bossart (2012, p. 4-19 to 4-20); 2. Aertsens et al. (2004, p. 37); 3. De Cannière et al. (2010, Table 5.3-1)
NA = not available

Table 14. Mineralogical: Composition

Property	Opalinus Clay	Boom Clay
Total clay (% total dry weight)	28 – 93[1]	30 – 60[2]
Illite (% total dry weight)	15.0 – 30.0[1]	10 – 45[2]
Chlorite (% total dry weight)	3.0 – 18.0[1]	0 – 5[2]
Kaolinite (% total dry weight)	15.0 – 37.0[1]	5 – 20[2]
Illite/smectite ML (% total dry weight)	5.0 – 20.0[1]	10 – 30[2]
Chlorite/smectite ML (% total dry weight)	NA	0 – 5[2]
Quartz (% total dry weight)	10.0 – 32.0[1]	15 – 60[2]
Feldspars – K (% total dry weight)	0.0 – 6.0[1]	1 – 10[2]
Feldspars – albite (% total dry weight)	0.0 – 2.0[1]	1 – 10[2]
Calcite (% total dry weight)	4.0 – 22.0[1]	1 – 5[2]
Dolomite/ankerite (% total dry weight)	0.0 – 1.0[1]	present[2]
Siderite (% total dry weight)	0.0 – 6.0[1]	present[2]
Pyrite (% total dry weight)	0.0 – 3.0[1]	1 – 5[2]
Gypsum (% total dry weight)	0.0 – 0.5[1]	NA
Organic Carbon (% total dry weight)	0.4 – 1.2[1]	1 – 5[2]

1. Bossart (2012, p. 4-12); 2. DeCraen et al. (2004, Table 1-2)
NA = not available

Table 15. Mineralogical: Cation Exchange Capacity (CEC)

Property	Opalinus Clay	Boom Clay
Total CEC (mEq/100 g rock)	9.44 – 13.35[1]	24.00[2]
Exchangeable Na (mEq/100 g rock)	3.61 – 6.37[1]	8.7[2]
Exchangeable K (mEq/100 g rock)	0.58 – 0.92[1]	2.3[2]
Exchangeable Ca (mEq/100 g rock)	2.25 – 3.58[1]	3.8[2]
Exchangeable Mg (mEq/100 g rock)	1.55 – 2.38[1]	3.7[2]
Exchangeable Sr (mEq/100 g rock)	0.10 – 0.36[1]	NA
Selectivity – log(Na/K)	0.7 – 0.84[3]	1.2[2]
Selectivity – log(Na/Mg)	0.0 – 2.0[3]	0.32[2]
Selectivity – log(Na/Ca)	4.0 to 22.0[3]	0.18[2]
Selectivity – log(Na/Sr)	0.0 – 1.0[3]	NA

1. Bossart (2012, p. 4-13); 2. Lolivier et al. (1998, Table II); 3. Pearson et al. (2010, Table 4)
NA = not available

Table 16. Mineralogical: Sorption Coefficients

Property	Opalinus Clay *	Boom Clay**
H(HTO) (m^3-kg^{-1})	0 - 0[1]	NA
C(inorg.) (m^3-kg^{-1})	0.0016 - 0.0016[1]	NA
C(org.) (m^3-kg^{-1})	0 - 0[1]	NA
Cl(-I) (m^3-kg^{-1})	0 - 0[1]	NA
Ca(II) (m^3-kg^{-1})	0.0002 - 0.0066[1]	NA
Co(II) (m^3-kg^{-1})	0.033 - 7.4[1]	NA
Ni(II) (m^3-kg^{-1})	0.080 - 10.8[1]	NA
Se(-II) (m^3-kg^{-1})	0 - 0[1]	NA
Sr(II) (m^3-kg^{-1})	0.0002 - 0.0066[1]	NA
Zr(IV) (m^3-kg^{-1})	0.56 - 214.0[1]	NA
Nb(V) (m^3-kg^{-1})	0.22 - 72.8[1]	NA
Mo(VI) (m^3-kg^{-1})	0.0011 - 0.257[1]	NA
Tc(IV) (m^3-kg^{-1})	8.79 - 349.0[1]	52.2 - 65.7[2]
Ru(III/IV) (m^3-kg^{-1})	0.33 - 75[1]	NA
Pd(II) (m^3-kg^{-1})	0.33 - 75[1]	NA
Ag(I) (m^3-kg^{-1})	0 - 0[1]	NA
Cd(II) (m^3-kg^{-1})	0.011 - 2.95[1]	NA
Sn(IV) (m^3-kg^{-1})	7.86 - 1540[1]	NA
Sb(III) (m^3-kg^{-1})	0.22 - 143.0[1]	NA
I(-I) (m^3-kg^{-1})	0 - 0.0005[1]	NA
Cs(I) (m^3-kg^{-1})	0.092 - 3.3[1]	NA
Ce(III) (m^3-kg^{-1})	9.49 - 377.0[1]	NA
Pm(III) (m^3-kg^{-1})	9.49 - 377.0[1]	NA
Sm(III) (m^3-kg^{-1})	9.49 - 377.0[1]	NA
Eu(III) (m^3-kg^{-1})	13.3 - 269.0[1]	0.32 - 12.6[2]
Ho(III) (m^3-kg^{-1})	9.49 - 377.0[1]	NA
Hf(IV) (m^3-kg^{-1})	0.55 - 213.6[1]	NA
Pb(II) (m^3-kg^{-1})	0.057 - 128.0[1]	NA
Po(IV) (m^3-kg^{-1})	0.013 - 2.52[1]	NA
Ra(II) (m^3-kg^{-1})	0.0001 - 0.0046[1]	NA
Ac(III) (m^3-kg^{-1})	2.07 - 139.0[1]	NA
Th(IV) (m^3-kg^{-1})	12.3 - 249.0[1]	0.69 - 21.8[2]
Pa(IV) (m^3-kg^{-1})	0.5 - 50[1]	NA
U(IV) (m^3-kg^{-1})	3.25 - 129.0[1]	NA
Np(IV) (m^3-kg^{-1})	8.79 - 349.0[1]	6.42 - 75.5[2]
Pu(III) (m^3-kg^{-1})	2.76 - 185.0[1]	12.8 - 37.0[2]
Am(III) (m^3-kg^{-1})	2.93 - 98.6[1]	0.86 - 21.8[2]
Cm(III) (m^3-kg^{-1})	2.07 - 139.0[1]	4.87 - 13.4[2]
Pa(V) (m^3-kg^{-1})	NA	0.84 - 233.2[2]
Pu(IV) (m^3-kg^{-1})	NA	176.9 - 387.0[2]

1. Bradbury and Baeyens (2003, Tables 7 and 9); 2. Maes et al. (2011, p. 1597)
NA = not available

* Bradbury and Baeyens (2003), Table 7 mean values divided or multiplied by the uncertainty factors in Bradbury and Baeyens (2003) Table 9
**Values computed from retardation factors using conversion given in Maes et al. (2011) Table 4 note a).

Gouy-Chapman theory is used to represent clay swelling effects that result from aqueous compositional changes (Liu et al., 2011, Section 4). This theory requires density of solid and aqueous phases (Tables 1 and 4), porosity (Table 1), volume fraction of swelling clay minerals (Table 14), exchangeable cations (Table 15), cation exchange capacity (Table 15), aqueous chemical composition (Table 10), the initial half-widths between swelling and non-swelling mineral platelets (Table 17), specific surface area (Table 17), and some general scientific parameters such as elementary electric charge and Boltzmann's constant (Table 18), and the dielectric constant of pore fluid (Table 4).

Table 17. Mineralogical: Additional Parameters for the Gouy-Chapman Model

Property	Opalinus Clay	Boom Clay
nondimensional midplane potential - nondimensional distance function parameter, *a* (for pure smectite)	1.81 – 3.54[1]	1.81 – 3.54[1]
nondimensional midplane potential - nondimensional distance function parameter, *b* (for pure smectite)	-4.13 to -3.17[1]	-4.13 to -3.17[1]
Basal half-spacing for swelling clay (A)	20 – 40[1]	20 – 40[1]
Basal half-spacing for non-swelling clay (A)	10[1]	10[1]
Specific surface area (m^2-g^{-1})	24 – 37 (BET); 112 – 147 (adsorption)[2]	44 (BET); 200 – 250 (adsorption)[3]

1. Liu et al. (2011, Table 4-2 and p. 91); 2. Bossart (2012, p. 4-17); 3. Mazurek et al. (2003, p. 160)

5. Thermal Model

The thermal model uses Fourier's theory for conductive heat transfer as well as convective heat transfer. This theory requires thermal conductivity for saturated and dry conditions, the dry bulk rock specific heat, and aqueous specific heat. Porosity and density of the rock and fractures, as well as the aqueous density are also needed for the thermal model, but these have already been discussed for the hydrological model. Thermal-mechanical coupling requires parameters for the thermal expansion of the rock and aqueous phase. Thermal properties are given in Table 18. The database needs to be able to accommodate spatial dependence of these parameters.

Table 18. Thermal: Conductive/Convective Heat Transfer and Thermal-Mechanical

Property	Opalinus Clay	Boom Clay
bulk rock thermal conductivity parallel to bedding ($W\text{-}m^{-1}\text{-}°C^{-1}$)	1.7 – 2.1[1,2]	1.35 – 1.7[3]
bulk rock thermal conductivity perpendicular to bedding ($W\text{-}m^{-1}\text{-}°C^{-1}$)	0.8 – 1.2[1,2]	
bulk rock specific heat ($J\text{-}kg^{-1}\text{-}°C^{-1}$)	860 – 920[1,2]	1402[4]
bulk rock thermal expansion coefficient ($°C^{-1}$)	1.5e-6 – 1.5e-5[1,2]	1e-5 – 5e-5[3]
aqueous specific heat ($J\text{-}kg^{-1}\text{-}°C^{-1}$) (at natural temperature – see Table 4)	4186 – 4188[5]	4185[5]
aqueous thermal conductivity ($W\text{-}m^{-1}\text{-}°C^{-1}$) (at natural temperature – see Table 4)	0.59[5]	0.59[5]
aqueous thermal expansion coefficient ($°C^{-1}$) (at natural temperature – see Table 4)	1.3e-4 – 1.5e-4[5]	1.6e-4[5]
moist air specific heat ($J\text{-}kg^{-1}\text{-}°C^{-1}$) (at natural temperature – see Table 4)	1.0e3[6]	1.0e3[6]
moist air thermal conductivity ($W\text{-}m^{-1}\text{-}°C^{-1}$) (at natural temperature – see Table 4)	2.5e-2[6]	2.5e-2[6]
thermal expansion coefficient ($°C^{-1}$) (dry air at 15° C)	3.48e-3[5]	3.48e-3[5]

1. Bossart (2012, p. 4-18); 2. Jobmann and Polster (2007, Table 2); 3. Li et al. (2007, Table 4.4); 4. Li et al. (2007, Tables 4.3 and 4.4 – volumetric heat capacity divided by bulk density) ; 5. Batchelor (1967, Appendix1); 6. Tsilingiris (2008, Figures 3 and 4)

6. Non-Site-Specific Parameters

Other parameters used for modeling of THMC processes are not site-specific. These parameters are summarized in table 19.

Table 19. Non-Site-Specific Parameters

Property	Value
gravitational acceleration ($m\text{-}s^{-2}$)	9.80[1]
molecular weight (kg)	molecule dependent
Boltzmann's constant ($J\text{-}°C^{-1}$)	1.38e-23[1]
elementary electric charge (coulombs (C))	1.60e-19[1]
permittivity of free space ($C^2\text{-}N^{-1}\text{-}m^{-2}$)	8.85e-12[1]

1. Reynolds and Perkins (1977, Table A4 and p. 9)

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